A Quick Review Of How To Set-Up & Run WRF-Chem 3.9.1.1

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WRF-Chem

- It is assumed that the user of WRF-Chem :
  - is ***very familiar*** with the WRF model system
  - have run WPS and a weather simulation using WRFV3
  - knows FORTRAN and can edit code, recompile, etc.

- The chemistry code is available from WRF web page.
  - Questions: Send email to WRF-Chem help (wrfchemhelp.gsd@noaa.gov)
  - Web page: https://ruc.noaa.gov/wrf/wrf-chem/

- Test data is available as well (tutorial exercises)
  - Small domain (41x41x31 grid points, 100 km horiz. spacing)

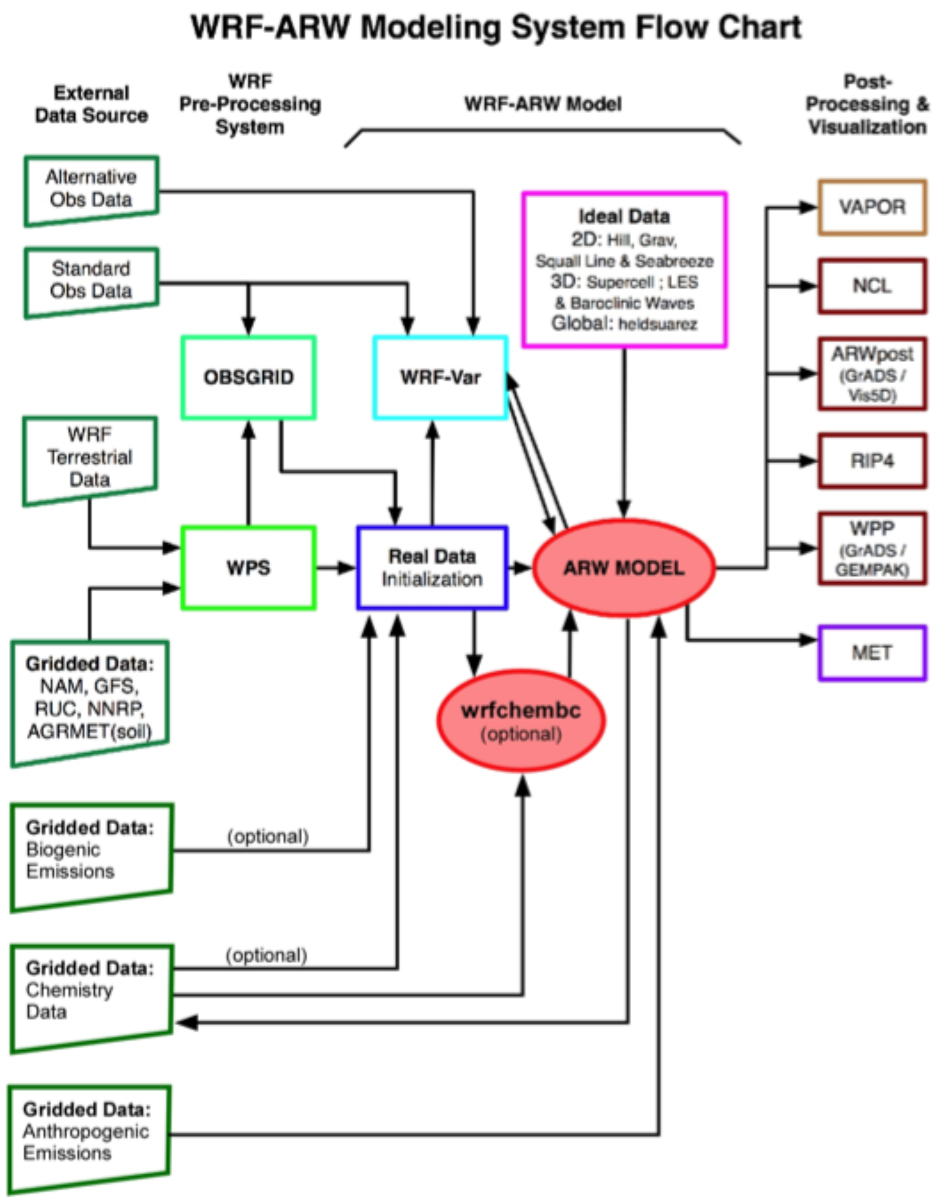
WRF-Chem

- GOAL: To understand how:
  - to make a WRF simulation that includes chemistry
    - Navigate all of the input choices and namelist options
- To accomplish this goal:
  - Learn steps to compile code,
  - Learn how to include emission sources,
    - Anthropogenic (US and global)
    - Biogenic
    - Biomass Burning
    - Dust
  - Learn about modifying initial and lateral boundary conditions
  - Become familiar with some namelist.input settings

WRF-Chem: Compile code

- Compile WRF-Chem code (already done for tutorial)
  - Set environment variables
    - Define which model core to build (use ARW only).
      - setenv EM_CORE 1
    - Chemistry code is to be included in the WRF model build
      - setenv WRF_CHEM 1
    - Kinetic Pre-Processor (KPP) code (if you want to run with a gas chemistry)
      - setenv WRF_KPP 1 => if KPP is to be included
      - setenv FLEX_LIB_DIR /usr/lib
      - setenv YACC '/usr/bin/yacc –d'
      - setenv WRF_KPP 0 => if KPP is NOT to be included
  - Configure and issue "compile em_real" command
    - Save compile output to file
    - Check results for errors and check known problems web page if no wrf.exe

WRF-Chem Emissions



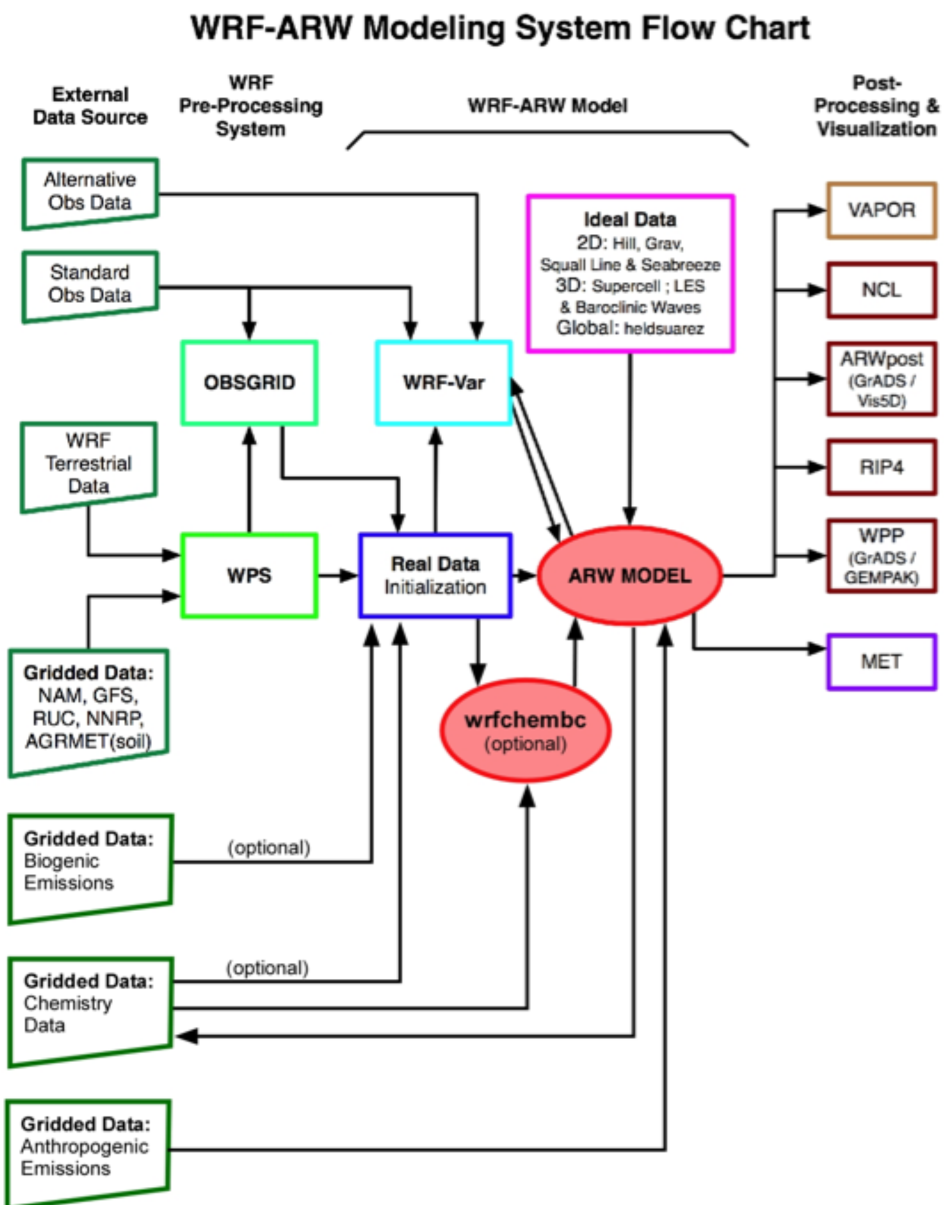
WRF-Chem Emissions

- Two sources of anthropogenic emissions available on WRF-Chem ftp site:
  - Global: RETRO (.5 degree, monthly) and EDGAR (1 degree, annual), HTAP (0.1 degree, monthly)
    - Run PREP_CHEM (Tutorial exercise)
  - EPA's National Emissions Inventory (NEI-2011) for U.S.
  - Both include programs to map to WRF grid; binary output files
- Can use other external emissions data
  - Start with "raw" emissions data
  - Specify the speciation for the desired chemical mechanism
  - Prepared the 3-D (or 2-D) anthropogenic emissions data set
    - Map data onto your WRF-Chem simulation domain
  - Output data
  - Goal: have data in a WRF data file to run with model

WRF-Chem Emissions

- The “available” methodology for emissions uses a convert program
  - Program called convert_emiss.exe (./compile emi_conv)
    - Reads header information from a WRF input file
    - Reads binary emissions data
    - Writes a netCDF data file that WRF-Chem can read
- convert_emiss is very simple. Uses just a few namelist settings.
  - emiss_opt=3 – NEI emissions for U.S.A.
  - emiss_opt=5 – RETRO/EDGAR or HTAP global emissions
- Data is read in via auxinput5 when running wrf.exe
  - auxinput5_inname = ‘wrfchemi_<hr>z_d<domain>, (optional)
  - io_form_auxinput5 = 2,
- Chpt. 3 and Appendix A of User’s Guide for more information
- Users can create input data files through any other methodology

WRF-Chem Biogenic Emissions



WRF-Chem
Biogenic Emissions

- 4 choices for Biogenic emissions
- Option 1: No biogenic emissions (bio_emiss_opt = 0):
  - You can provide biogenic emissions through anthropogenic input.
  - No additional input data files.

- Option 2 (bio_emiss_opt = 1):
  - Landuse based emissions following Guenther et al (1993, 1994), Simpson et al. (1995). Emissions depends on both temperature and photosynthetic active radiation.
  - No additional input data files.
  - Small number of vegetation types (errors?)

WRF-Chem
Biogenic Emissions

- Option 3 (bio_emiss_opt = 2): (mostly used for the US domain)
  - User specified from external data source
    - Biogenic Emissions Inventory System (BEIS) version 3.14 [*Vukovich and Pierce*, 2002] with land-use obtained from the Biogenic Emissions Landuse Database version 3 (BELD3) [*Pierce et al*., 1998].
  - Static 2-D surface data provided in input data file and are modified according to the environment
  - Data is read in via auxinput6 when running real.exe
    - auxinput6_inname = 'wrfbiochemi_d01',
    - io_form_auxinput6 = 2,

WRF-Chem
Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN (best choice?!)
  - Separate program made available by NCAR
  - Global data with base resolution of ~ 1 km
    - Leaf Area Index, vegetation type, emission factors
  - Steps:
    1. Download MEGAN code from the NCAR web-page
    2. megan_bio_emiss.tar
       - megan.data.tar.
         (when uncompressed ~ 28 GB)

https://www2.acom.ucar.edu/modeling/model-emissions-gases-and-aerosols-nature-megan

WRF-Chem
Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN
  - Steps:

    2. Compile megan_bio_emiss

    3. Create wrfbiochemi_d01 data file using:
       - wrfinput,
       - RAW MEGAN data files,
       - settings in megan_bio_emiss.input file
       - About 10 Gb of memory

WRF-Chem
Biogenic Emissions

- Option 4 (bio_emiss_opt = 3): MEGAN
  - Steps:

    4. View wrfbiochemi_d01 data file to verify data is correct

    5. Run real.exe and wrf.exe
       - Add ne_area setting to the WRF chemistry namelist!!!
         » ne_area = number of chemical species in chem_opt

One of the tutorial exercises to test this namelist options

https://www2.acom.ucar.edu/modeling/model-emissions-gases-and-aerosols-nature-megan

WRF-Chem Biomass Burning Emissions

- 2 choices for biomass burning emissions
- Option 1: No biomass emissions (biomass_burn_opt = 0):
  - No additional input data files.
- Option 2 (biomass_burn_opt = 1):
  - Use prep_chem_sources program to read WFABBA, or MODIS data
  - Convert binary data to wrffirechemi_d01 input file
  - Data read in through auxinput7 when running real.exe

WRF-Chem Dust Emissions

- 4 choices for dust emissions
- Option 1: No dust emissions (dust_opt = 0):
  - No additional input data files.
- Option 2 (dust_opt = 1):
  - Need to include surface erosion data in WPS
  - Use new GEOGRID table for running geogrid.exe
  - Dust data included in wrfinput file
- Option 3 (dust_opt = 3)
  - AFWA scheme uses same method as option 2
- Option 4 (dust_opt = 4)
  - Univ. of Cologne (Germany) dust scheme
  - Needs to have additional sediment lofting option set (see User's Guide)
- Work tutorial exercise Dust for more information.

WRF-Chem
GOCART Background Data

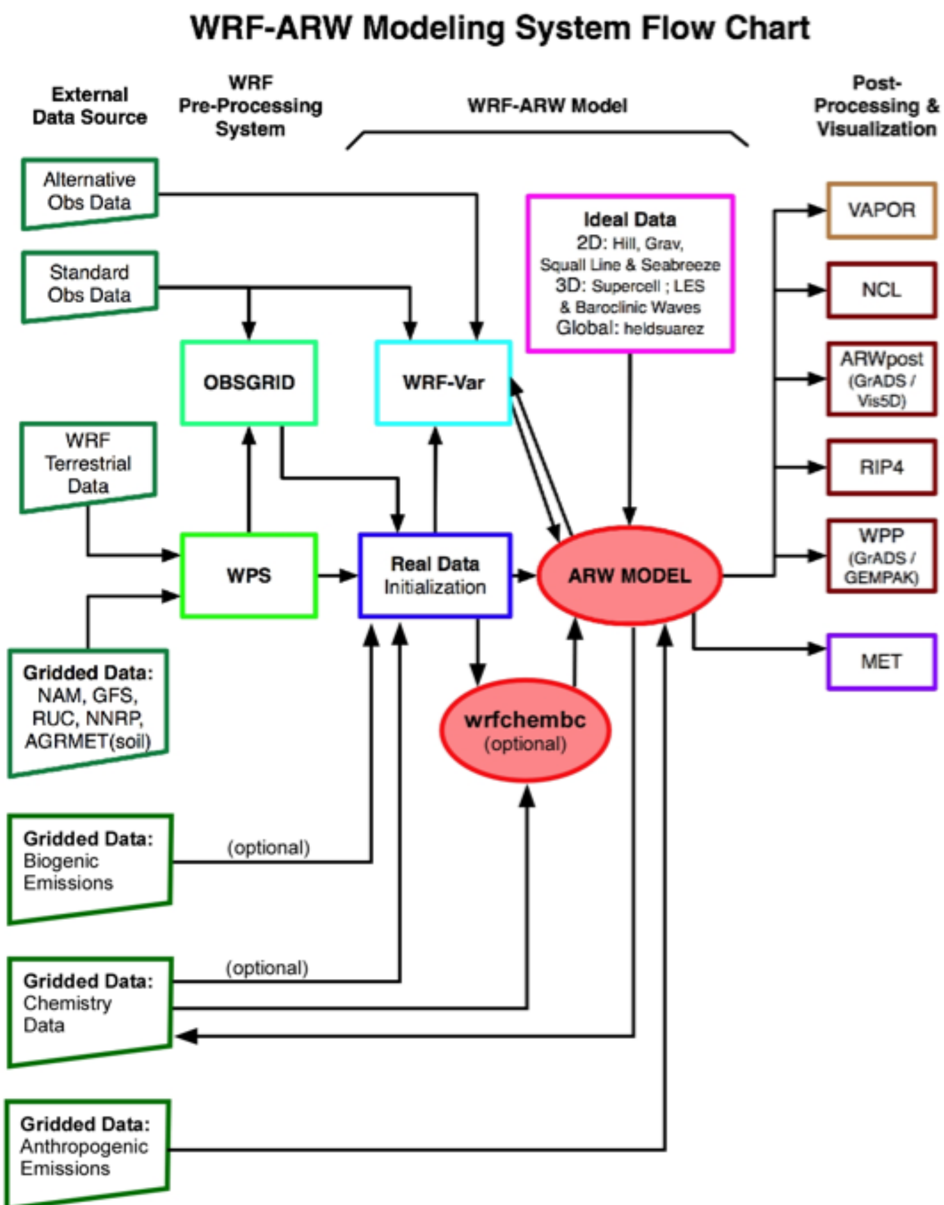
- Includes DMS, SO2, H2O2
  - From running prep_chem_sources with GOCART included
  - Planned to be moved to WPS in future

- Run prep_chem_sources program to produce external binary data files

- Convert binary data files to WRF input files
  - chem_opt = 300 or 301 and/or dmsemis_opt=1

- Data read by real.exe through auxinput8
  - File name wrfchemi_gocart_bg_d01

WRF-Chem Boundary Conditions



WRF-Chem Chemistry B.C.s

- External tools under development to provide global model data as BC and initial conditions

- Test program available: wrfchembc (Rainer Schmitz - Univ. of Chile)
  - Available code runs with MPI-MATCH & RAQMS data
  - Adds lateral boundary data for chemical species to wrfbdy_d01
  - User specifies which chemical species to use
    - Need to choose chemical species from global model
    - Need to speciate global model data for WRF-Chem chemistry
    - Requires knowledge from user regarding chemistry (not turn-key)
- wrfinput_d01 not modified
  - Can result in differences near boundaries at start of simulation

WRF-Chem Chemistry B.C.s

- Other groups are exploring other possible ways to generate input/B.C. data for WRF-Chem
  - NCAR has a program available if using MOZART. MOZBC sets space and time-varying chemical initial (IC) and boundary conditions (BC)
  - global model output (MOZART-4 or CAM-Chem)

MOZBC : http://www.acd.ucar.edu/wrf-chem/download.shtml

MOZART data (2004-2008):

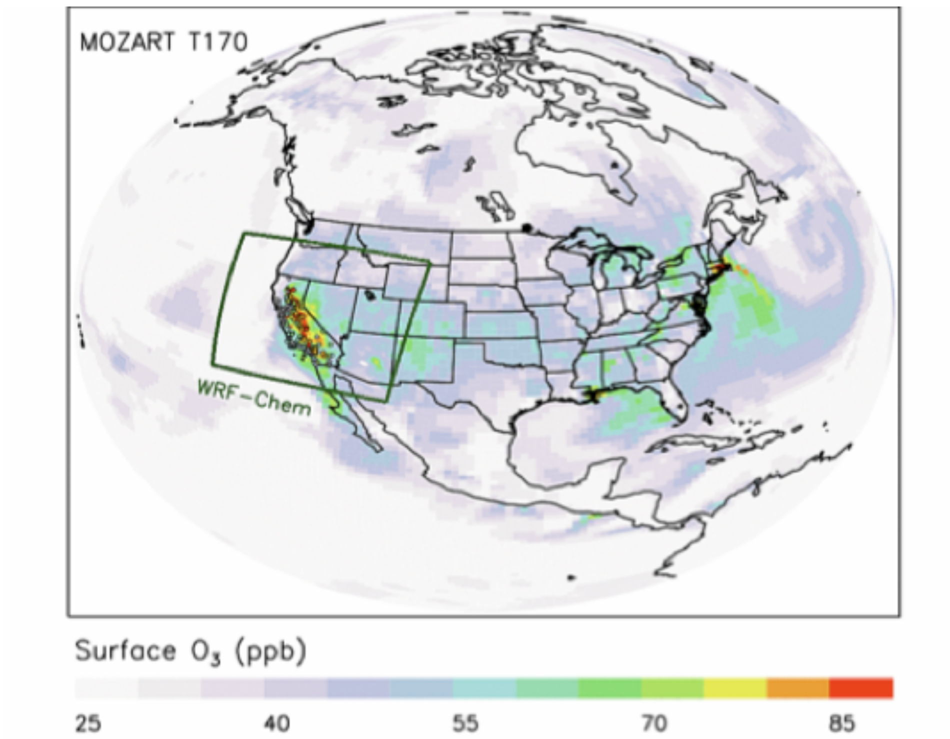
http://www.acd.ucar.edu/wrf-chem/mozart.shtml

https://www2.acom.ucar.edu/wrf-chem

- Note: MOZART/CAM-Chem data are interpolated only in space.

WRF-Chem Chemistry B.C.s

- Program will fill the chemical fields in your wrfinput_d<nn> and wrfbdy_d<nn> files with global model output.



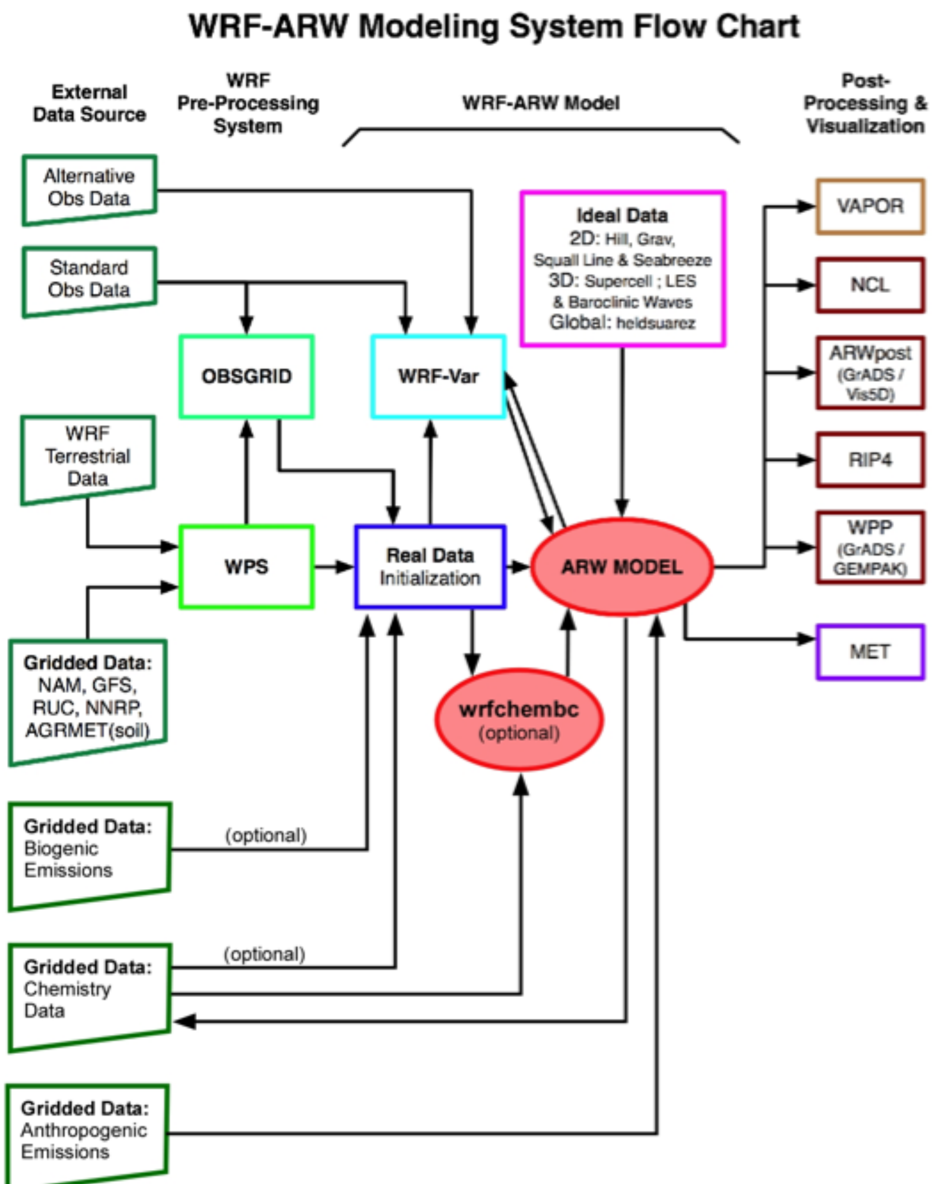
- To enable chemical IC and BC when running WRF-Chem set in namelist.input:
  have_bcs_chem = .true.

WRF-Chem Chemistry B.C.s

- What if you have different GCM data?
- Methodology is the same
    - Read global model chemistry data
    - Skip over if not a desired chemistry species
    - Determine grid point location on WRF-Chem grid
    - If at boundary, interpolate data to WRF-Chem grid
    - Once completed reading/interpolating global data:
        - Open wrfbdy_d01 data file
        - Write boundary data to wrfbdy_d01

Some WRF-Chem users have been able to run mozbc to read CO2 data from Carbon Tracker.

WRF-Chem Namelist



WRF-Chem Namelist

- **Time control namelist options**

- A few of the chemistry related namelist options
  - More details provided in Chapter 4 of User’s Guide

WRF-Chem Namelist

- Time control namelist
  - Chemistry input fields come in through auxiliary input ports
  - Biogenic emissions use auxinput 6 for example

```
&time_control
…
auxinput6_inname        = ‘wrfbiochemi_d<domain>,
auxinput6_interval_m    = 1440,
io_form_auxinput6       = 2,
```

Recall:
Defining a variable-set for an I/O stream

- **Fields are added to a variable-set on an I/O stream at compile-time with Registry**

```
#       Type  Sym  Dims   Use     Tlev  Stag   IO         Dname   Descrip
state   real  u    ikjb   dyn_em  2     X      i01rhusdf  "U"     "X WIND COMPONENT“
```

IO is a string that specifies if the variable is to be subject to initial, restart, or history I/O. The string may consist of '**h**' (subject to history I/O), '**i**' (initial dataset), or '**r**' (restart dataset). The 'h', 'r', and 'i' specifiers may appear in any order or combination.

The ‘h’ and ‘i’ specifiers may be followed by an optional integer string consisting of ‘0’, ‘1’, … , ‘9’ Zero denotes that the variable is part of the principal input or history I/O stream. The characters ‘1’ through ‘9’ denote one of the auxiliary input or history I/O streams.

WRF-Chem Registry

- Thus, in registry.chem

```
state   real    -          i+jf     emis_ant    -       -     -      -                   "Anthropogenic Emissions"        ""
state    real  e_iso        i+jf     emis_ant    1        Z      i5r    "E_ISO"             "Isoprene EMISSIONS"  "mol km^-2 hr^-1"
state    real  e_so2        i+jf     emis_ant    1        Z      i5r    "E_SO2"             "EMISSIONS"         "mol km^-2 hr^-1"
state    real  e_no         i+jf     emis_ant    1        Z      i5r    "E_NO"              "EMISSIONS"         "mol km^-2 hr^-1”

#
state    real  e_bio        ijo     misc        1        Z      r       "E_BIO"           "EMISSIONS"           "ppm m/min"
state    real  sebio_iso     ij      misc        1        -      i6r     "sebio_iso"       "Reference biog emiss"  "mol km^-2 hr^-1"
state    real  sebio_oli     ij      misc        1        -      i6r     "sebio_oli"       "Reference biog emiss"  "mol km^-2 hr^-1”

# additional arrays needed for biomass burning emissions input
state    real    -            i]jf      ebu_in     -       -       -       -                  "Biomass burnung input "        ””
state    real  ebu_in_no        i]jf      ebu_in     1       -       i{7}     "ebu_in_no"          "EMISSIONS"         "mol km^-2 hr^-1”
state    real  ebu_in_co        i]jf      ebu_in     1       -       i{7}     "ebu_in_co"          "EMISSIONS"         "mol km^-2 hr^-1”

# Input for GOCART: Background chemistry, erodible surface emissions map
state    real  backg_oh      ikj     misc       1       -      i8r    "BACKG_OH"      "Background OH "      "volume mixing ratio"
state    real  backg_h2o2     ikj     misc       1       -      i8r    "BACKG_H2O2"     "Background H2O2"     "volume mixing ratio”
```

WRF-Chem Namelist

- For the chemistry variables to come in via auxiliary port
  - Registry set for input via auxiliary port

Auxiliary port number	Description
5	Anthropogenic emissions
6	Biogenic emissions
7	Surface biomass burning data
8	GOCART background fields
12	External chemistry fields (wrfout data from previous run)
13	Volcanic Ash emissions
14	Aircraft emissions
15	Green House Gas emissions

WRF-Chem Namelist

- For the chemistry variables to come in via auxiliary ports (cont.)
  - Namelist set in time_control

```
&time_control
…
auxinput6_inname = 'wrfbiochemi_d01',
auxinput7_inname = 'wrffirechemi_d<domain>',
auxinput8_inname = 'wrfchemi_gocart_bg_d<domain>',
auxinput12_inname = 'wrf_chem_input',
auxinput13_inname = 'wrfchemv_d<domain>',
auxinput5_interval_m = 86400, 86400, 60,
auxinput7_interval_m = 86400, 86400, 60,
auxinput8_interval_m = 86400, 86400, 60,
auxinput13_interval_m = 86400, 86400, 60,
io_form_auxinput2 = 2,
io_form_auxinput5 = 2,
io_form_auxinput6 = 0,
io_form_auxinput7 = 0,
io_form_auxinput8 = 0,
io_form_auxinput12 = 0,
io_form_auxinput13 = 0,
```

WRF-Chem Namelist

A few of the chemistry namelist options

- More details provided in Chapter 4 of WRF-Chem User's Guide

WRF-Chem Namelist

- Chemistry control namelist

Chem_opt	Description
0	No chemistry
1 - 40	Chemical mechanisms (RADM2, CBMZ), tracer options (chem_opt=13 to 17)
101 - 200	Options covering RADM2, RACM, CBMZ, MOZART, SAPRC99, NMHC9 chemical mechanisms using KPP.
300 – 303	GOCART aerosol options
400 – 403	Dust and Volcano options (volcanic and surface lofted)
501 – 504	CBMZ and MAM aerosols (run with CAM5 physics)

WRF-Chem Namelist

emiss_opt	Description
0	no anthropogenic emissions
2	use radm2 anthropogenic emissions
3	use radm2/MADE/SORGAM anthropogenic emissions
4	use CBMZ/MOSAIC anthropogenic emissions
5	GOCART RACM_KPP emissions
6	GOCART simple emissions
7	MOZART emissions .
8	MOZCART (MOZART + GOCART aerosols) emissions
13	SAPRC99 emissions
16	CO2 tracer emissions
17	Green House Gas emissions

Remember: emiss_opt sets emissions structure (registry.chem)

#emission package definitions

package eradmsorg emiss_opt==3
emis_ant:e_iso,e_so2,e_no,e_no2,e_co,e_eth,e_hc3,e_hc5,e_hc8,e_xyl,e_ol2,e_olt,e_oli,e_tol,e_csl,e_hcho,e_ald,e_ket,e_ora2,e_nh3,e_pm25i,e_pm25j,e_pm_10,e_eci,e_ecj,e_orgi,e_orgj,e_so4i,e_so4j,e_no3i,e_no3j,e_naaj,e_naai,e_orgi_a,e_orgj_a,e_orgi_bb,e_orgj_bb

package ecptec emiss_opt==5
emis_ant:e_iso,e_so2,e_no,e_no2,e_co,e_eth,e_hc3,e_hc5,e_hc8,e_xyl,e_ol2,e_olt,e_oli,e_tol,e_csl,e_hcho,e_ald,e_ket,e_ora2,e_nh3,e_pm_25,e_pm_10,e_oc,e_sulf,e_bc

Anthropogenic CO2, CO and CH4 emissions:

package eco2 emiss_opt==16 emis_ant:e_co2,e_co2tst,e_co

package eghg emiss_opt==17 emis_ant:e_co2,e_co2tst,e_co,e_cotst,e_ch4,e_ch4tst

WRF-Chem Namelist

cu_rad_feedback	Description
.false.	No feedback from the parameterized convection to the atmospheric radiation and the photolysis schemes. (logical)
.true.	Feedback from the parameterized convection to the radiation schemes turned on. (logical) - use Grell cumulus scheme
progn	
0	Turns off prognostic cloud droplet number in the Lin et al. microphysics
1	Prognostic cloud droplet number included in the Lin et al. This effectively turns the Lin et al. and Morrison schemes into a second-moment microphysical scheme. If set with chem._opt=0 a default prescribed aerosol concentration is used. *You can test these options during the practice sessions.*

WRF-Chem Namelist

cldchem_onoff	Description
0	cloud chemistry turned off in the simulation, also see the “chem_opt” parameter
1	cloud chemistry turned on in the simulation, also see the “chem_opt” parameter
wetscav_onoff	
0	wet scavenging turned off in the simulation, also see the “chem_opt” parameter
1	wet scavenging turned on in the simulation, also see the “chem_opt” parameter

Any Questions?

NAMELIST CHOICES

Dust only

```
&chem
chem_opt                  = 401,
chemdt                    = 5,
dust_opt                  = 1
/
```

NAMELIST CHOICES

GOCART (simple)

```
&time_control
 io_form_auxinput5 = 2,
 io_form_auxinput6 = 0,
 io_form_auxinput7 = 2,
 io_form_auxinput8 = 2,
/
```

```
&chem
 kemit = 1,
 chem_opt = 300,
 chemdt = 60,
 io_style_emissions = 1,
 emiss_opt = 5,
 dust_opt = 1,
 seas_opt = 1,
 biomass_burn_opt = 1,
 plumerisefire_frq = 30,
 aer_ra_feedback = 1,
 aer_op_opt = 1,
 opt_pars_out = 1,
/
```

NAMELIST CHOICES

RACM-SOA_VBS

(Exercise)

```
&time_control
 io_form_auxinput5          = 2,
 io_form_auxinput6          = 2,
 io_form_auxinput7          = 2,
 io_form_auxinput8          = 2,
/
```

```
&chem
chem_opt                    = 108,
 chemdt                     = 0,
 gas_drydep_opt             = 1,
 aer_drydep_opt             = 1,
 bio_emiss_opt              = 3,
 ne_area                    = 104,
 wetscav_onoff              = -10,
 cldchem_onoff              = 0,
vertmix_onoff               = 1,
chem_conv_tr                = 1,
 conv_tr_wetscav            = 1,
 conv_tr_aqchem             = 1,
seas_opt                    = 0,
 dust_opt                   = 0,
aer_op_opt                  = 0,
/
```

Tutorial exercises

cd /sysdisk1/Chem_exercises_2018

```
Exercise_aerosol_radiation_cloud_interactions/
Exercise_dust/
Exercise_Global_Emissions_RACM_GOCART/
Exercise_megan_bio_emiss/
Exercise_mozbc/
Exercise_RACM_KPP_SOA/
Exercise_RACM_KPP_SOA_megan_bio_emiss/
Exercise_RACM_KPP_SOA_restart/
Exercise_US_Emissions/
Exercise_volcanic_ash/
Exercise_WRFChem_DART_localization/
```

Exercises – day 1

- Exercise_dust – Mediterranean domain, run WPS and WRF-Chem3.9.1.1, various dust flux options (dust_opt=1,3,4) with dust chemistry option (chem_opt=401)

- Exercise_Global_Emissions_RACM_GOCART – Mediterranean domain, run the prep_chem tool with global HTAP (0.1x0.1 degrees) anthropogenic emissions and biogenic, and biomass burning emissions; GOCART background fields; Chemistry option RACM_KPP_GOCART, full gas chemistry+simple aerosols

- Exercise_mozbc – generating boundary conditions for the Mediterranean domain using the MOZART global model output

- Exercise_volcanic_ash – chem_opt=400

US Emissions and chemistry Exercises

1. Exercise_US_Emissions
2. Exercise_RACM_KPP_SOA
3. Exercise_RACM_KPP_SOA_restart (this can be skipped)
4. Exercise_megan_bio_emiss
5. Exercise_RACM_KPP_SOA_megan_bio_emiss

Follow this order

More advanced Exercises (Day 2)

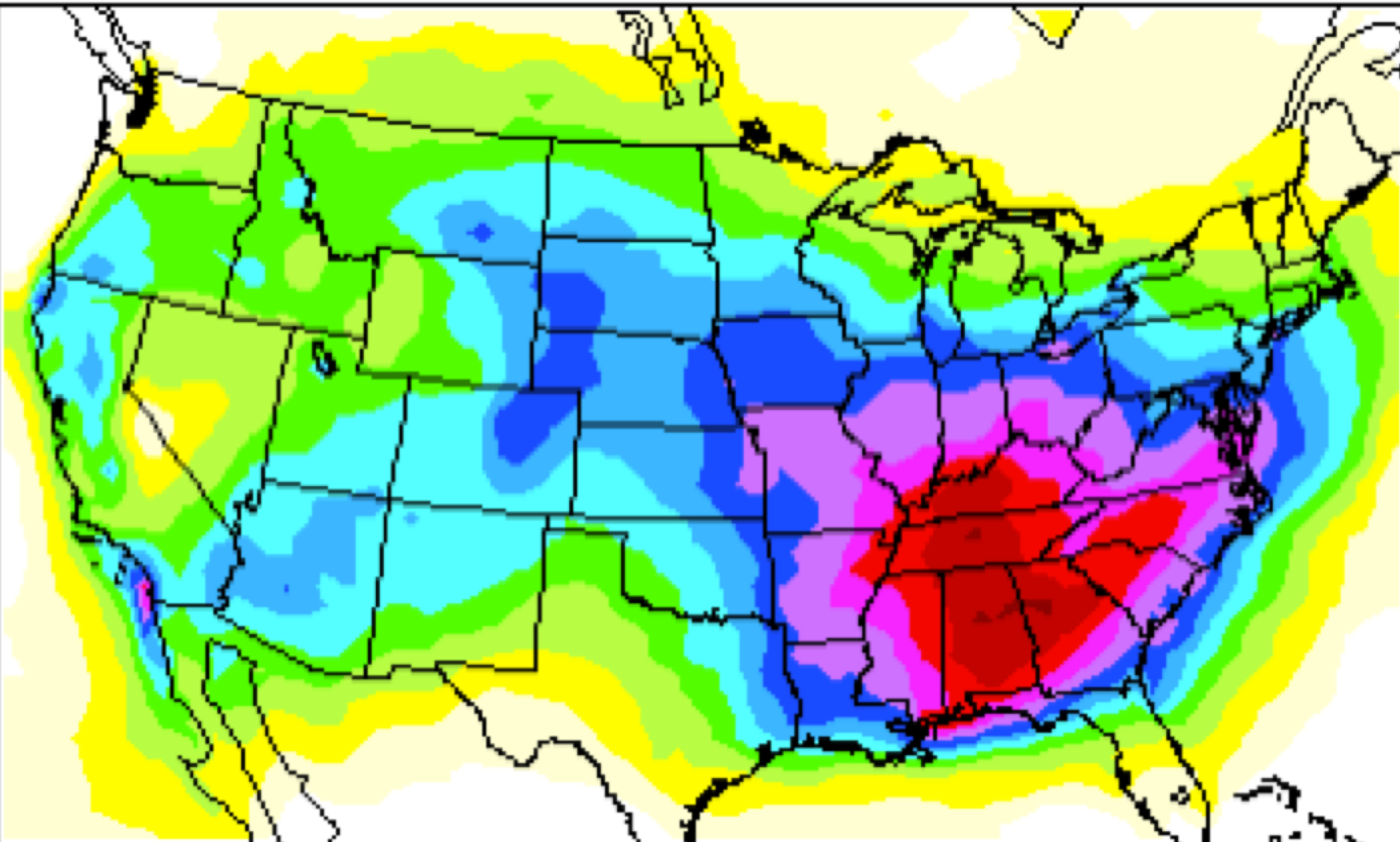
- Exercise_aerosol_direct_indirect_forcing - Running WRF-Chem with aerosol direct and indirect forcing with full gas, aerosol and aqueous chemistry using the RACM_SOA_VBS_AQCHEM (chem_opt=109) option

- Exercise_WRFChem_DART_Localization – chemical data assimilation exercise by A.Mizzi (NCAR)

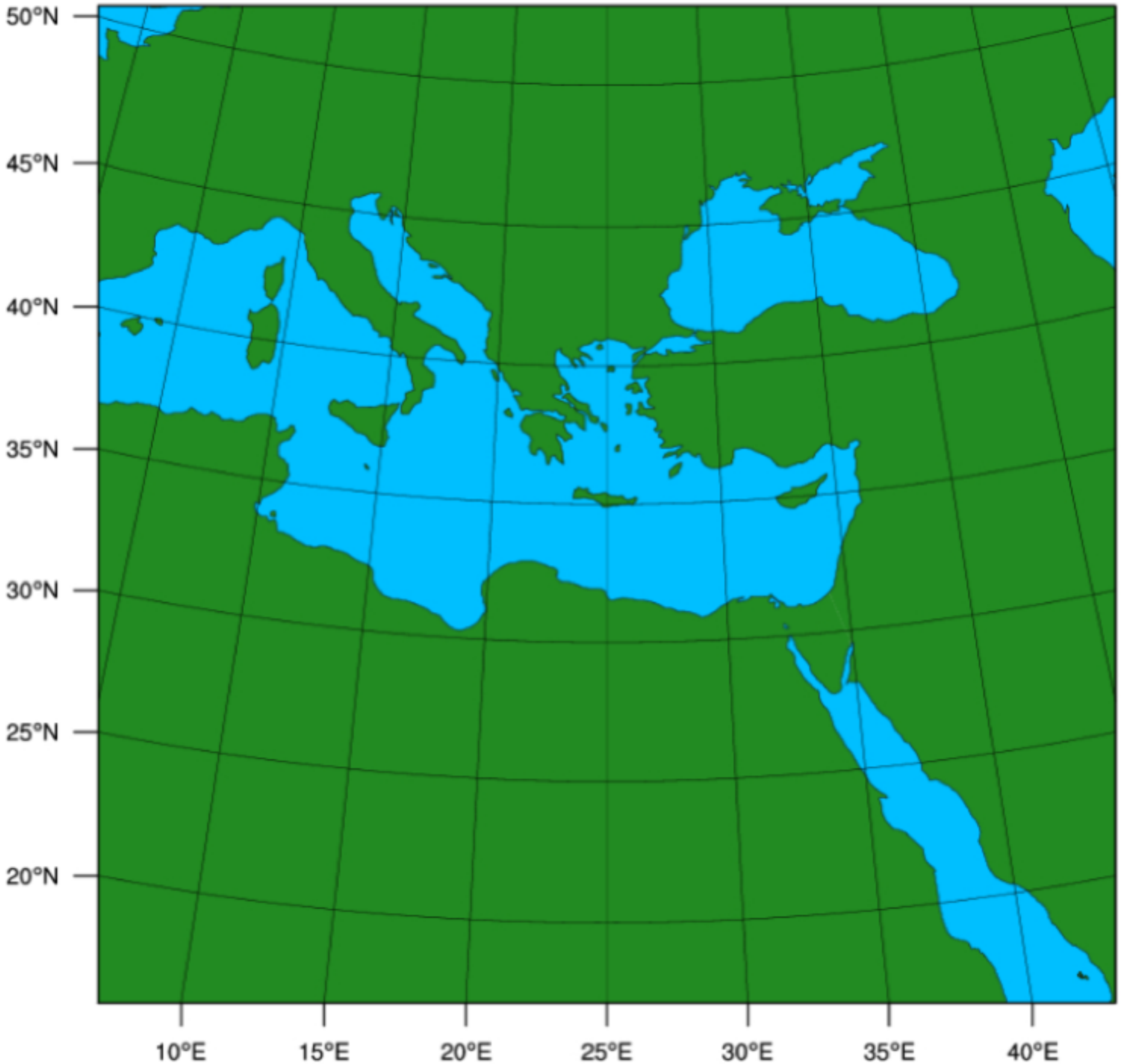
Exercises

- There are Run_* directories and Exercise_* directories on your computer.
- The Exercise_* folders contain instructions.txt, input and namelist files to run the exercise.
- First exercise to work on: Exercise_dust
- You will run all the programs in Run_* folders. You will need to copy all the necessary input data and namelist files to your Run_* directory.
- Enjoy☺️

CONUS domain, 60km resolution



Mediterranean domain, 100km resolution



Questions?